Using OpenMP

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Outline

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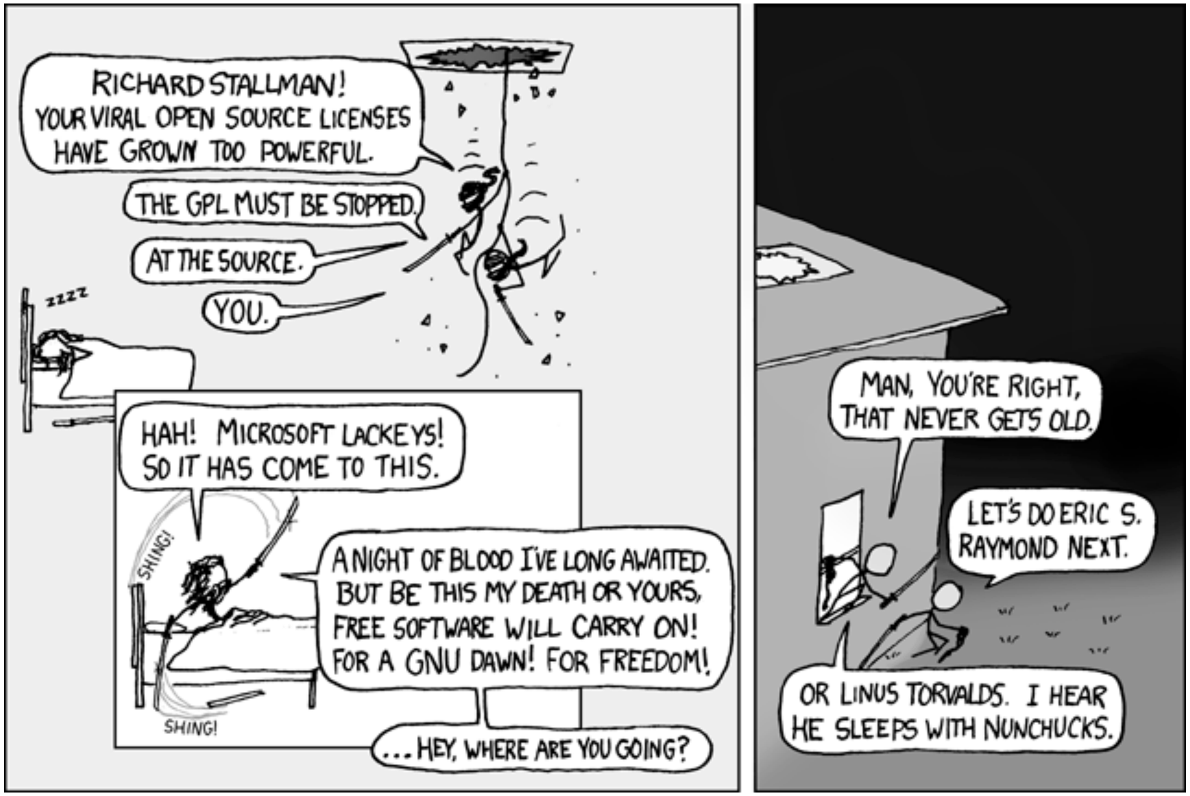


I. ABOUT OPENMP

Source: http://xkcd.com/225/

About OpenMP

- Industry-standard shared memory programming model
- Developed in 1997
- OpenMP Architecture Review Board (ARB) determines additions and updates to standard

Advantages to OpenMP

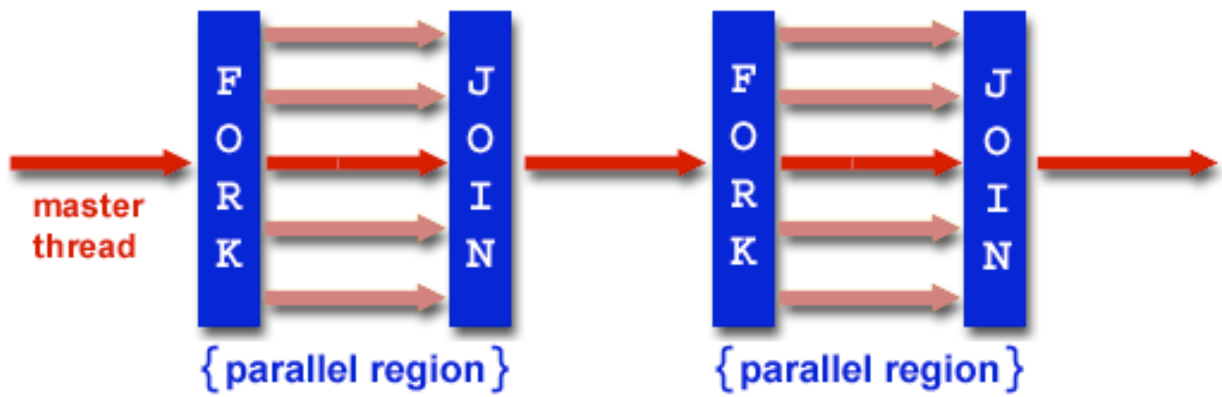
- Parallelize small parts of application, one at a time (beginning with most time-critical parts)
- Can express simple or complex algorithms
- Code size grows only modestly
- Expression of parallelism flows clearly, so code is easy to read
- Single source code for OpenMP and non-OpenMP – non-OpenMP compilers simply ignore OMP directives

OpenMP Programming Model

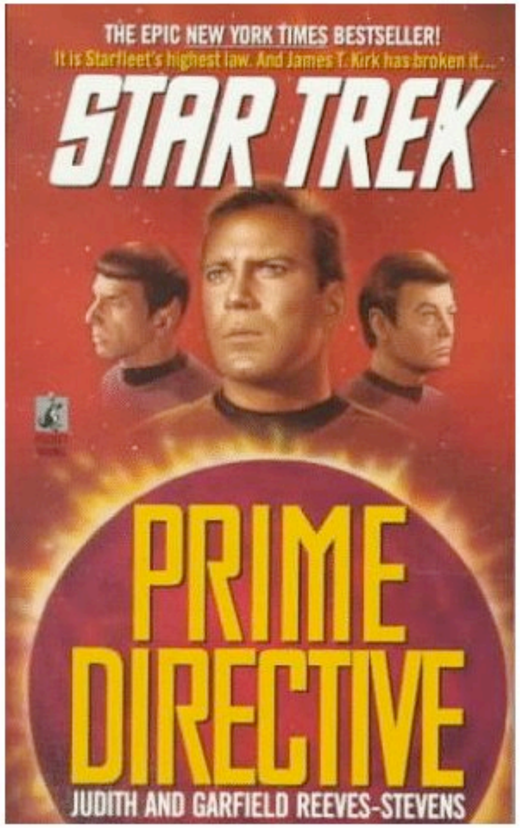
- Application Programmer Interface (API) is combination of
  - Directives
  - Runtime library routines
  - Environment variables
- API falls into three categories
  - Expression of parallelism (flow control)
  - Data sharing among threads (communication)
  - Synchronization (coordination or interaction)

Parallelism

- Shared memory, thread-based parallelism
- Explicit parallelism (parallel regions)
- Fork/join model



Source: https://computing.llnl.gov/tutorials/openMP/



II. OPENMP DIRECTIVES

Star Trek: Prime Directive **by Judith and Garfield Reeves-Stevens, ISBN 0671744666**

II. OpenMP Directives

- Syntax overview
- Parallel
- Loop
- Sections
- Synchronization
- Reduction

Syntax Overview: C/C++

- Basic format

  `#pragma omp directive-name [clause] newline`

- All directives followed by newline
- Uses pragma construct (pragma = Greek for “thing”)
- Case sensitive
- Directives follow standard rules for C/C++ compiler directives
- Long directive lines can be continued by escaping newline character with \

Syntax Overview: Fortran

- Basic format:

  `sentinel directive-name [clause]`

- Three accepted sentinels: `!$omp` `*$omp` `c$omp`
- Some directives paired with `end` clause
- Fixed-form code:
  - Any of three sentinels beginning at column 1
  - Initial directive line has space/zero in column 6
  - Continuation directive line has non-space/zero in column 6
  - Standard rules for fixed-form line length, spaces, etc. apply
- Free-form code:
  - `!$omp` only accepted sentinel
  - Sentinel can be in any column, but must be preceded by only white space and followed by a space
  - Line to be continued must end in `&` and following line begins with sentinel
  - Standard rules for free-form line length, spaces, etc. apply

OpenMP Directives: Parallel

- A block of code executed by multiple threads
- Syntax:

```
#pragma omp parallel private(list)\
  shared(list)
{
   /* parallel section */
}

!$omp parallel private(list) &
!$omp shared(list)
! Parallel section
!$omp end parallel
```

Simple Example (C/C++)

```
#include <stdio.h>
#include <omp.h>
int main (int argc, char *argv[]) {
  int tid;
  printf("Hello world from threads:\n");
  #pragma omp parallel private(tid)
  {
   tid = omp_get_thread_num();
   printf("<%d>\n", tid);
  }
  printf("I am sequential now\n");
  return 0;
}
```

Simple Example (Fortran)

```
program hello
integer tid, omp_get_thread_num
write(*,*) 'Hello world from threads:'
!$OMP parallel private(tid)
tid = omp_get_thread_num()
write(*,*) '<', tid, '>'
!$omp end parallel
write(*,*) 'I am sequential now'
end
```

Output (Simple Example)

Output 1

```
Hello world from
  threads:
<0>
<1>
<2>
<3>
<4>
I am sequential now
```

Output 2

```
Hello world from
  threads:
<1>
<2>
<0>
<4>
<3>
I am sequential now
```

Order of execution is scheduled by OS!!!!!!

OpenMP Directives: Loop

- Iterations of the loop following the directive are executed in parallel
- Syntax:

```
#pragma omp for schedule(type [,chunk]) \
private(list) shared(list) nowait
 {
   /* for loop */
 }

!$OMP do schedule(type [,chunk]) &
!$OMP private(list) shared(list)
C do loop goes here
!$OMP end do nowait
```

  - *type* = {`static`, `dynamic`, `guided`, `runtime`}
  - If `nowait` specified, threads do not synchronize at end of loop

Which Loops Are Parallelizable?

Parallelizable

- Number of iterations known upon entry, and does not change
- Each iteration independent of all others
- No data dependence

Not Parallelizable

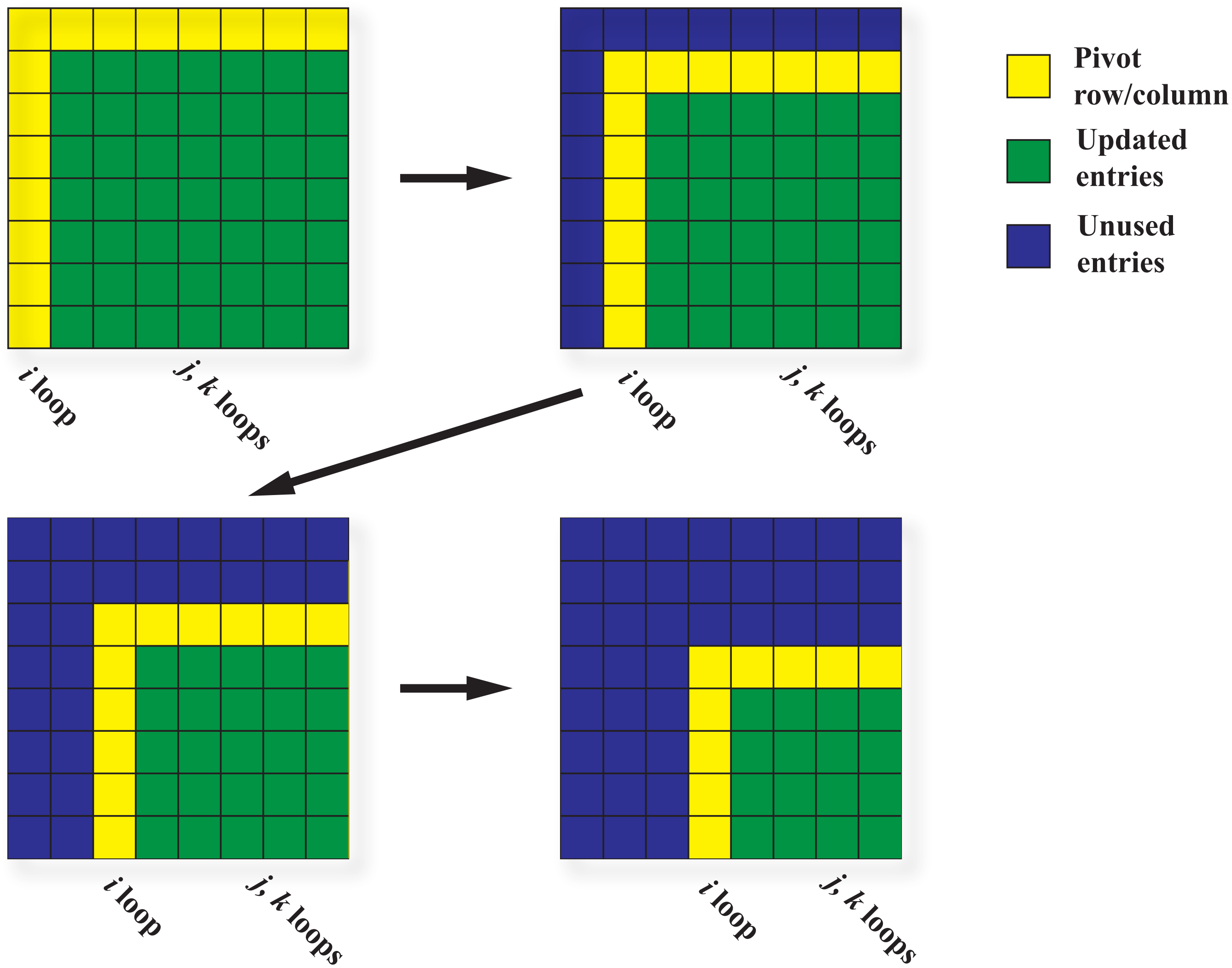
- Conditional loops (many while loops)
- Iterator loops (e.g., iterating over a `std::list<…>` in C++)
- Iterations dependent upon each other
- Data dependence

Example: Parallelizable?

```
/* Gaussian Elimination (no pivoting):
   x = A\b                                    */

for (int i = 0; i < N-1; i++) {
  for (int j = i; j < N; j++) {
    double ratio = A[j][i]/A[i][i];
    for (int k = i; k < N; k++) {
      A[j][k] -= (ratio*A[i][k]);
      b[j] -= (ratio*b[i]);
    }
  }
}
```

Example: Parallelizable?



Example: Parallelizable?

- Outermost Loop (`i`):
  - `N-1` iterations
  - Iterations depend upon each other (values computed at step `i-1` used in step `i`)
- Inner loop (`j`):
  - `N-i` iterations (constant for given `i`)
  - Iterations can be performed in any order
- Innermost loop (`k`):
  - `N-i` iterations (constant for given `i`)
  - Iterations can be performed in any order

Example: Parallelizable?

```
/* Gaussian Elimination (no pivoting):
   x = A\b                                */

for (int i = 0; i < N-1; i++) {
#pragma omp parallel for
  for (int j = i; j < N; j++) {
    double ratio = A[j][i]/A[i][i];
    for (int k = i; k < N; k++) {
      A[j][k] -= (ratio*A[i][k]);
      b[j] -= (ratio*b[i]);
    }
  }
}
```

Note: can combine `parallel` and `for` into single `pragma` line

OpenMP Directives: Loop Scheduling

- Default scheduling determined by implementation
- Static
  - ID of thread performing particular iteration is function of iteration number and number of threads
  - Statically assigned at beginning of loop
  - Load imbalance may be issue if iterations have different amounts of work
- Dynamic
  - Assignment of threads determined at runtime (round robin)
  - Each thread gets more work after completing current work
  - Load balance is possible

Loop: Simple Example

```
#include <omp.h>
#define CHUNKSIZE 100
#define N     1000
int main ()  {
  int i, chunk;
  float a[N], b[N], c[N];
  /* Some initializations */
  for (i=0; i < N; i++)
    a[i] = b[i] = i * 1.0;
  chunk = CHUNKSIZE;
  #pragma omp parallel shared(a,b,c,chunk) private(i)
  {
    #pragma omp for schedule(dynamic,chunk) nowait
    for (i=0; i < N; i++)
      c[i] = a[i] + b[i];
  }  /* end of parallel section */
  return 0;
}
```

OpenMP Directives: Sections

- Non-iterative work-sharing construct
- Divide enclosed sections of code among threads
- Section directives nested within sections directive
- Syntax: C/C++

```
#pragma omp sections
{
  #pragma omp section
  /* first section */
  #pragma omp section
  /* next section */
}
```

Fortran

```
!$OMP sections

!$OMP section
C First section
!$OMP section
C Second section
!$OMP end sections
```

Sections: Simple Example

```
#include <omp.h>
#define N     1000
int main () {
  int i;
  double a[N], b[N],
   c[N], d[N];
  /* Some initializations
   */
  for (i=0; i < N; i++) {
    a[i] = i * 1.5;
    b[i] = i + 22.35;
  }
```

```
  #pragma omp parallel \
   shared(a,b,c,d) private(i)
  {
    #pragma omp sections nowait
    {
      #pragma omp section
        for (i=0; i < N; i++)
          c[i] = a[i] + b[i];
      #pragma omp section
        for (i=0; i < N; i++)
         d[i] = a[i] * b[i];
     }  /* end of sections */
   }  /* end of parallel section */
return 0;
}
```

OpenMP Directives: Synchronization

- Sometimes, need to make sure threads execute regions of code in proper order
  - Maybe one part depends on another part being completed
  - Maybe only one thread need execute a section of code
- Synchronization directives
  - Critical
  - Barrier
  - Single

OpenMP Directives: Synchronization

- **Critical**
  - Specifies section of code that must be executed by only one thread at a time
  - Syntax: C/C++

    ```
    #pragma omp critical [name]
    ```

    Fortran

    ```
    !$OMP critical [name]
    !$OMP end critical
    ```
  - Names are global identifiers – critical regions with same name are treated as same region
- **Single**
  - Enclosed code is to be executed by only one thread
  - Useful for thread-unsafe sections of code (e.g., I/O)
  - Syntax: C/C++

    ```
    #pragma omp single
    ```

    Fortran

    ```
    !$OMP single
    !$OMP end single
    ```

OpenMP Directives: Synchronization

- **Barrier**
  - Synchronizes all threads: thread reaches barrier and waits until all other threads have reached barrier, then resumes executing code following barrier
  - Syntax: C/C++ | Fortran

    ```
    #pragma omp barrier        !$OMP barrier
    ```
  - Sequence of work-sharing and barrier regions encountered must be the same for every thread

OpenMP Directives: Reduction

- **Reduces list of variables into one, using operator (e.g., max, sum, product, etc.)**
- **Syntax**

```
#pragma omp reduction(op : list)
!$OMP reduction(op : list)
```

where ***list*** is list of variables and ***op*** is one of following:

– C/C++: **+**, **-**, *****, **&**, **^**, **|**, **&&**, or **||**

– Fortran: **+**, **-**, *****, **.and.**, **.or.**, **.eqv.**, **.neqv.**, or **max**, **min**, **iand**, **ior**, **ieor**

III. VARIABLE SCOPE

Angled spotting scope. Source: http://www.spottingscopes.us/angled-scope-328.jpg

Variable Scope

- By default, all variables shared except
  - Certain loop index values – private by default
  - Local variables and value parameters within subroutines called within parallel region – private
  - Variables declared within lexical extent of parallel region – private

Default Scope Example

```
void caller(int *a, int n) {
int i,j,m=3;
#pragma omp parallel for
for (i=0; i<n; i++) {
  int k=m;
  for (j=1; j<=5; j++) {
    callee(&a[i], &k, j);
  }
}
void callee(int *x, int *y, int
   z) {
  int ii;
  static int cnt;
  cnt++;
  for (ii=1; ii<z; ii++) {
    *x = *y + z;
  }
}
```

Var	Scope	Comment
a	shared	Declared outside parallel construct
n	shared	same
i	private	Parallel loop index
j	shared	Sequential loop index
m	shared	Declared outside parallel construct
k	private	Automatic variable/parallel region
x	private	Passed by value
*x	shared	(actually a)
y	private	Passed by value
*y	private	(actually k)
z	private	(actually j)
ii	private	Local stack variable in called function
cnt	shared	Declared static (like global)

Variable Scope

- Good programming practice: explicitly declare scope of all variables
- This helps you as programmer understand how variables are used in program
- Reduces chances of data race conditions or unexplained behavior

Variable Scope: Shared

- Syntax
  - `shared(`*`list`*`)`
- One instance of shared variable, and each thread can read or modify it
- WARNING: watch out for multiple threads simultaneously updating same variable, or one reading while another writes
- Example

```
#pragma omp parallel for shared(a)
for (i = 0; i < N; i++) {
  a[i] += i;
}
```

Variable Scope: Shared – Bad Example

```
#pragma omp parallel for shared(n_eq)
for (i = 0; i < N; i++) {
  if (a[i] == b[i]) {
    n_eq++;
  }
}
```

- `n_eq` will not be correctly updated
- Instead, put `n_eq++;` in critical block (slow); introduce private variable `my_n_eq`, then update `n_eq` in critical block after loop (faster); or use `reduction` pragma (best)

Variable Scope: Private

- Syntax
  - `private(list)`
- Gives each thread its own copy of variable
- Example

```
#pragma omp parallel private(i, my_n_eq)
{
  #pragma omp for
  for (i = 0; i < N; i++) {
    if (a[i] == b[i])  my_n_eq++;
  }
  #pragma omp critical (update_sum)
  {
    n_eq+=my_n_eq;
  }
}
```

Best Solution for Sum

```
#pragma parallel for
  reduction(+:n_eq)
for (i = 0; i < N; i++) {
  if (a[i] == b[i]) {
    n_eq = n_eq+1;
  }
}
```

IV. RUNTIME LIBRARY ROUTINES AND ENVIRONMENT VARIABLES

Mt. McKinley National Monument, July, 1966. Source: National Park Service Historic Photograph Collection, http://home.nps.gov/applications/hafe/hfc/npsphoto4h.cfm?Catalog_No=hpc-001845

OpenMP Runtime Library Routines

- `void omp_set_num_threads(int num_threads)`

  `subroutine omp_set_num_threads(scalar_integer_expression)`
  - Sets number of threads used in next parallel region
  - Must be called from serial portion of code

OpenMP Runtime Library Routines

- `int omp_get_num_threads()`

  `integer function omp_get_num_threads()`

  - Returns number of threads currently in team executing parallel region from which it is called

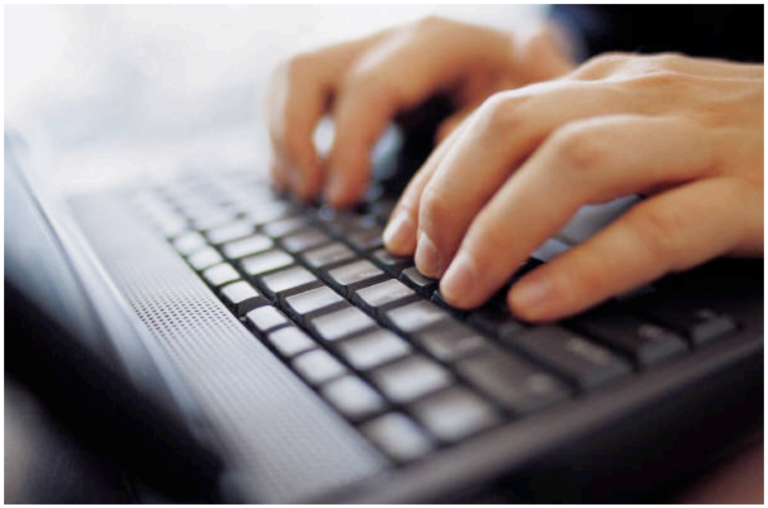
- `int omp_get_thread_num()`

  `integer function omp_get_thread_num()`

  - Returns rank of thread
  - `0 ≤ omp_get_thread_num() < omp_get_num_threads()`

OpenMP Environment Variables

- Set environment variables to control execution of parallel code
- `OMP_SCHEDULE`
  - Determines how iterations of loops are scheduled
  - E.g., `setenv OMP_SCHEDULE "guided, 4"`
- `OMP_NUM_THREADS`
  - Sets maximum number of threads
  - E.g., `setenv OMP_NUM_THREADS 4`



V. USING OPENMP

Conditional Compilation

- Can write single source code for use with or without OpenMP
- Pragmas/sentinels are ignored
- What about OpenMP runtime library routines?
  - `_OPENMP` macro is defined if OpenMP available: can use this to conditionally include `omp.h` header file, else redefine runtime library routines

Conditional Compilation

```
#ifdef _OPENMP
  #include <omp.h>
#else
  #define omp_get_thread_num() 0
#endif
…
int me = omp_get_thread_num();
…
```

Compiling Programs with OpenMP Directives on Jaguar and Kraken

- Compiler flags:
  - `-mp=nonuma` (PGI)
  - `-fopenmp` (GNU)
  - `-mp` (Pathscale)
- Many libraries already compiled with OpenMP directives
- Libsci
  - 10.3: link with `-lsci_quadcore_mp`
  - 10.2: link with `-lsci_mp`

Running Programs with OpenMP Directives on Jaguar and Kraken

- Set environment variable `OMP_NUM_THREADS` in batch script
- Use the depth (`-d`) in aprun command to represent number of threads per MPI process, and `-N` for number of MPI processes per node
- Example: to run on 64 quad-core nodes on Jaguar with 1 MPI process and 4 threads/MPI process, add the following to your script requesting 256 procs:

```
export OMP_NUM_THREADS=4
aprun -n 64 -N 1 -d 4 myprog
```

More about aprun

- `-n` *`pes`*
  - Allocates *`pes`* processing elements (PEs, think MPI tasks)
- `-N` *`pes_per_node`*
  - Specifies number of processing elements to place per node
  - Reducing number of PEs per node makes more resources available per PE
- `-d` *`depth`*
  - Allocates number of CPUs to be used by each PE and its threads (default 1)
  - If you set `OMP_NUM_THREADS` but do not specify depth, all threads will be allocated on a single core
- *`pes * pes_per_node * depth`* ≤ Number in PBS header

Bibliography/Resources: OpenMP

- Chapman, Barbara, Gabrielle Jost, and Ruud van der Pas. (2008) *Using OpenMP*, Cambridge, MA: MIT Press.
- Kendall, Ricky A. (2007) *Threads R Us*, http://www.nccs.gov/wp-content/training/scaling_workshop_pdfs/threadsRus.pdf
- LLNL OpenMP Tutorial, https://computing.llnl.gov/tutorials/openMP/